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Towards adaptive graph neural networks via solving prior-data conflicts

Key words: Graph neural networks; Heterophily; Prior-data conflict

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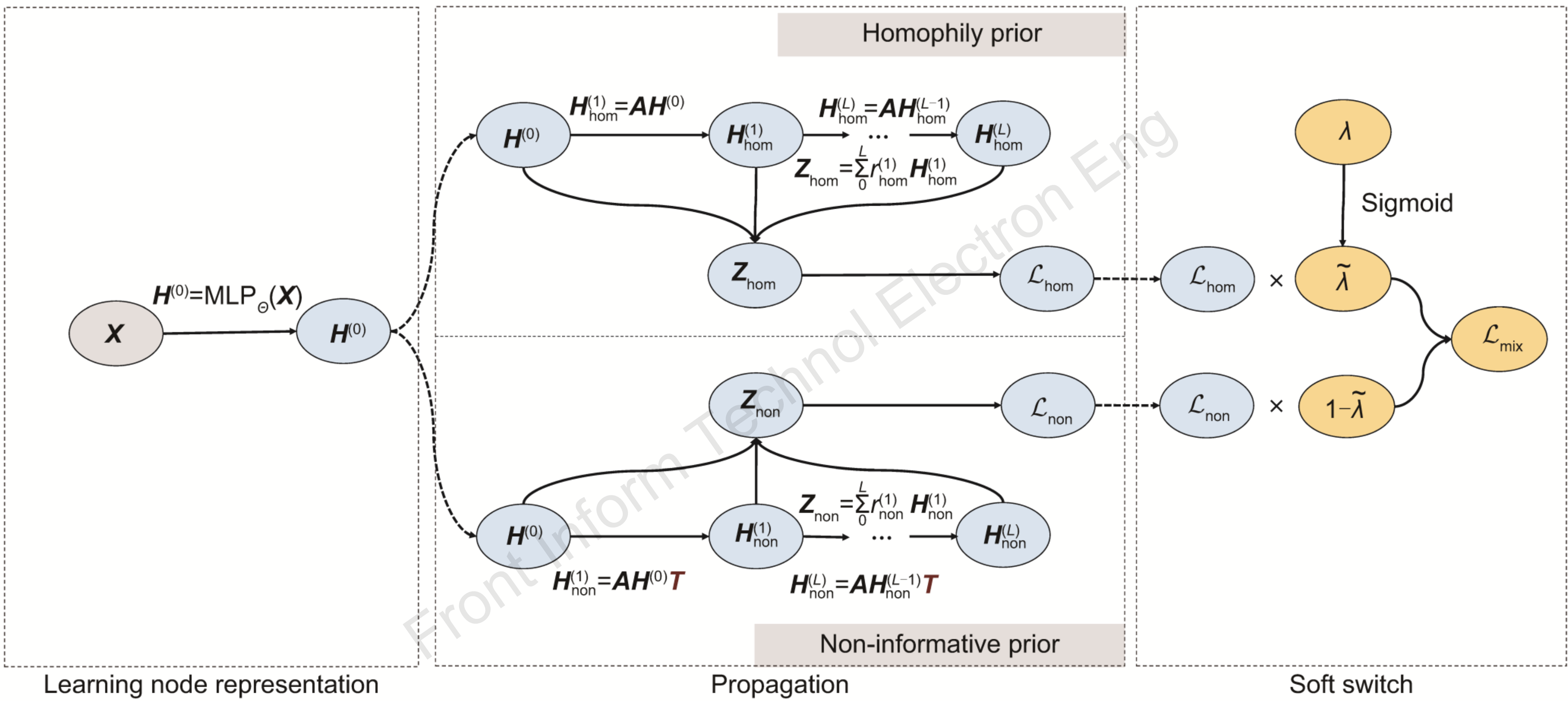
Motivation

- There is a key prior in the design of most graph neural network (GNN) models, the homophily prior, which posits that nodes with similar features or labels of the same class are more likely to be connected in the graph. The homophily prior provides a strong regularization that prevents GNN models from overfitting when the amount of training data is limited.
- However, graphs in the real world can be heterophilic.
  The mismatch between the prior knowledge and the data characteristics leads to suboptimal GNN performance in heterophilic settings. In some cases, even a multilayer perceptron (MLP) model could outperform most existing GNNs.

Main idea

- To address the prior-data conflicts of GNNs in heterophilic settings, we incorporate a noninformative prior in the model by formulating the relationship between connected nodes.
- We adopt a scheme of mixture priors and implement a soft switch module to adjust the weight of the priors according to the characteristics of the graphs. Such a design allows the model to converge quickly to the proper prior.
- Combining these two designs, we propose the mixture-prior GNN (MPGNN) model and evaluate it on both synthetic and real-world benchmarks.

Framework



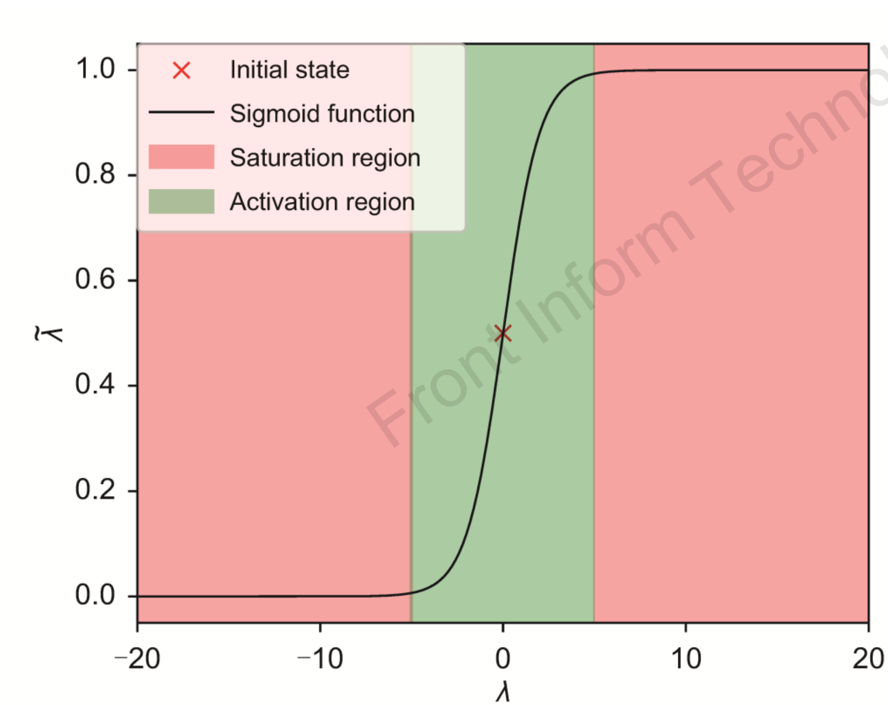
The overall framework of MPGNN. First, we use an MLP to obtain the representation of each node. After that, the node representations are propagated with two priors separately: homophily prior and non-informative prior. Finally, a soft switch is used to combine their results according to the characteristics of the graph.

Method

- Instead of following the homophily prior, we learn the inter-node relationships by formulating the transition probability as a latent variable *T* and integrating it into the propagation process.
- By optimizing the transition probability and the model parameters alternatively, MPGNN can capture the relationships between connected nodes in the graph, thus eliminating the prior-data conflict that is inherent in traditional GNNs in heterophilic settings.

Method

To avoid the performance drop when applying non-informative prior to homophilic graphs, we design a soft switch to select a suitable prior according to the graph characteristics adaptively.



The sigmoid soft switch. In the early training stage, the soft switch lies in the activation region. When the soft switch turns into the saturation region, gradient vanishing happens and the soft switch stops learning.

Major results

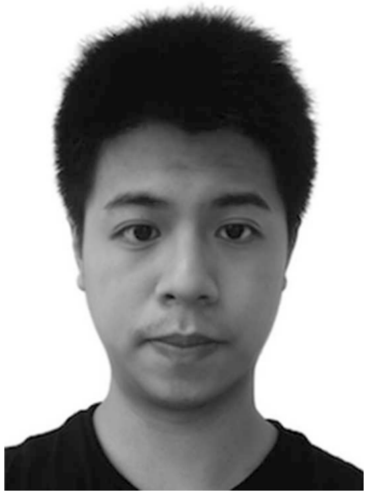
Table 1 Results for cSBM under sparse splitting

Model	Accuracy (%)								
	$\phi=-1.00$	$\phi=-0.75$	$\phi=-0.50$	$\phi=-0.25$	$\phi=0$	$\phi=0.25$	$\phi=0.50$	$\phi=0.75$	$\phi=1.00$
MPGNN	**97.96±0.76**	**96.37±0.55**	**94.92±1.04**	**62.98±2.19**	59.23±1.42	67.81±1.03	84.60±1.25	**94.60±0.67**	**95.40±1.08**
GPR-GNN	89.26±0.58	88.49±1.26	67.50±0.52	58.30±1.09	58.09±0.74	67.65±1.33	84.65±0.75	93.86±0.53	95.02±1.03
APPNP	49.60±0.21	51.52±0.26	56.08±0.31	59.10±0.49	60.34±1.07	**68.01±1.57**	**85.65±1.52**	94.24±0.48	92.82±0.63
MLP	50.03±0.94	53.13±0.48	56.28±0.62	59.25±0.49	**62.03±0.74**	60.48±0.59	57.81±0.37	53.23±0.21	50.31±0.28
GCN	55.88±0.50	62.54±0.75	56.32±0.44	52.33±0.51	54.38±0.32	67.03±0.35	84.38±0.20	93.34±1.53	83.64±0.58
GAT	53.44±0.32	57.70±0.51	53.19±0.39	51.55±0.35	53.36±0.63	63.38±0.15	81.03±0.35	88.65±0.41	82.08±0.33
JKNet	51.41±0.40	58.32±0.30	52.66±0.71	50.63±0.15	52.30±0.25	65.66±0.38	84.61±0.15	93.01±0.60	90.63±0.41

The highest accuracies are in bold

Conclusions

In this work, we demonstrate that the suboptimal performance of GNNs on heterophilic graphs is due to prior-data conflicts. We propose MPGNN, which solves such conflicts via (1) integrating a non-informative prior and (2) using a soft switch to balance the homophily prior and non-informative prior adaptively. With these two designs, MPGNN achieves state-of-the-art performance on both homophilic and heterophilic graphs.



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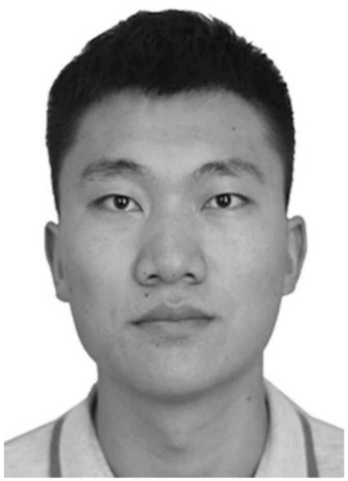

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